

# CHEMISTRY

## A **European** Journal

### Supporting Information

#### **Quantum Mechanical and Experimental Validation that Cyclobis(paraquat-*p*-phenylene) Forms a 1:1 Inclusion Complex with Tetrathiafulvalene**

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# CHEMISTRY

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### $\pi$ - $\pi$ Charge-Transfer Interactions: Comparisons of Theoretical Calculations with Experiment

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### Supporting Information

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## S1. Single Crystal X-Ray Crystallography

A single crystal of **Rt•4PF<sub>6</sub>** was grown from a mixture of *trans* and *cis* isomers in MeCN by vapour diffusion of diisopropyl ether at room temperature.

*Crystal data for Rt •4PF<sub>6</sub>*: C<sub>40</sub>H<sub>56</sub>O<sub>6</sub>S<sub>4</sub>, P<sub>4</sub>F<sub>24</sub>, C<sub>6</sub>H<sub>14</sub>O, C<sub>36</sub>H<sub>32</sub>N<sub>4</sub>, 3(C<sub>2</sub>H<sub>3</sub>N), green plate, *Mr* = 2086.96, crystal size 0.215 × 0.167 × 0.016 mm, triclinic, space group *P* $\bar{1}$ , *a* = 11.2281(4), *b* = 13.1328(5), *c* = 19.9925(9) Å,  $\alpha$  = 77.125(3),  $\beta$  = 85.321(3),  $\gamma$  = 65.056(3)°, *V* = 2605.57(18) Å<sup>3</sup>, *Z* = 1,  $\rho_{\text{calc}}$  = 1.330, *T* = 100(2) K,  $R_1(F^2 > 2\sigma F^2)$  = 0.0851,  $wR_2$  = 0.2094. Out of 17405 reflections a total of 8480 were unique. Crystallographic data (excluding structure factors) for the structures reported in this communication have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC–960538.

## S2. Coordinates of TTF ⊂ CBPQT<sup>4+</sup> Inclusion and Side-On Complexes

The geometries of TTF ⊂ CBPQT<sup>4+</sup> complexes were optimised at the level of M06-2X/6-311G\*\* with PCM model for MeCN ( $r_{\text{probe}}$  = 2.19 Å,  $\epsilon_{\text{optical}}$  = 1.81 and  $\epsilon_{\text{static}}$  = 37.5), as provided by the manual of Jaguar 7.9.<sup>[1]</sup> M06-2X functional is recommended for applications involving main group elements.<sup>[2]</sup> For TD-DFT calculations, a dense grid NRAD=125 was used to describe S atoms. Both geometry optimization and TD-DFT were carried out with GAMESS.

### S2.1 TTF ⊂ CBPQT<sup>4+</sup> Inclusion Complex-2CH<sub>3</sub>CN

M06-2X/6-311G\*\* in PCM: -3698.3894603666

M06-2X/6-311G(2df,p) in PCM: -3698.5435122102

H	0.1871455803	6.3297678835	0.5683544941
H	-0.8111526726	6.0410262299	2.0038433506
H	-0.5113302940	4.2355699283	3.2759593960
C	0.2185261216	3.7962720323	2.6117038507
H	4.3353096346	1.3233397983	1.1008091104
H	5.2964729846	-0.9404771302	1.3955053919
H	0.7322030052	2.1523352130	3.8494833300
N	0.4369873340	4.4540282429	1.4564588691
H	5.2671375120	-2.9875706001	2.2723630856
C	0.9110001822	2.6410736754	2.9016462866
C	3.7739731325	0.5774304697	1.6475514348
C	4.3268538812	-0.6770272041	1.7964870162
H	4.0364683187	-3.4563671002	3.4584660814
C	1.3466888165	4.0154465415	0.5714356093
C	1.8367360757	2.1415587539	1.9804778860
C	2.0654728536	2.8644533729	0.8095030357
C	2.5221083632	0.8496062673	2.2054348264
H	1.4891263033	4.5914201276	-0.3331277299
H	2.7683468730	2.5524883471	0.0485447741
N	3.6796367457	-1.6383447891	2.4805203603
C	1.8976232980	-0.1543083235	2.9476681597
H	0.9315015795	-0.0078531989	3.4090099175

C	2.4940970418	-1.3899683303	3.0629458380
C	-0.4416799669	5.6023413688	1.0788101787
H	2.0271676049	-2.2069223829	3.5964183756
C	4.1978456183	-3.0401987656	2.4652720807
C	-1.5499699748	5.0802252456	0.1951212096
H	-0.4323887087	5.3338716519	-1.6339761167
C	3.4602569047	-3.8052054024	1.3923705682
H	-2.9485476668	4.7848304150	1.8054931977
H	4.8955612284	-3.3667015729	-0.1520287026
H	1.8969089667	-4.4885982793	2.7117144135
C	-1.3369127007	4.9467813292	-1.1768677480
C	-2.7511955398	4.6407728198	0.7484645726
C	3.9307270250	-3.8053725318	0.0800939334
C	2.2527265047	-4.4348486250	1.6882977700
C	-2.2843187823	4.3170781377	-1.9719573658
C	-3.7019466613	4.0085144242	-0.0502088920
C	3.1630327429	-4.3620577647	-0.9391620789
C	1.4890416586	-4.9938511748	0.6723184620
H	-2.1038318739	4.2222793639	-3.0369631820
H	-4.6342849206	3.6666838314	0.3860032153
H	3.5361727616	-4.3528397450	-1.9583879107
C	-3.4551779534	3.8124464425	-1.4077741514
H	0.5517233035	-5.4789957796	0.9210574648
C	1.9213801833	-4.9264764253	-0.6509937482
C	-4.3866691099	2.9716358973	-2.2509037943
H	-2.8157881227	2.0869989265	-4.1210604273
C	0.9990288951	-5.3669472710	-1.7634982761
C	-2.9184660150	1.3411936899	-3.3450469819
N	-3.7999921873	1.6028046069	-2.3631485690
H	-4.4900313941	3.3569737804	-3.2637427661
H	1.2542668406	-3.4629182106	-3.5091533568
C	-2.1968680358	0.1683956459	-3.3513051688
H	-5.3750992550	2.8687948460	-1.8070519298
C	-4.0123907527	0.7102877382	-1.3805124114
H	-1.5140471669	0.0087644948	-4.1731000254
C	0.3599947062	-3.2986565474	-2.9223901749
N	0.0375613639	-4.2561071667	-2.0364640420
H	-4.7391135625	0.9830493406	-0.6259131935
C	-2.3729133694	-0.7669834828	-2.3251060159
C	-0.4157894921	-2.1665206071	-3.0580724058
C	-3.3270249773	-0.4857421319	-1.3422054795
C	-1.5533477342	-2.0002751134	-2.2611069198
H	-0.0892729521	-1.4228622641	-3.7721037287
C	-1.0633451904	-4.1359130572	-1.2736859887
H	-3.5247126256	-1.1525563341	-0.5105884565
H	-1.2724891423	-4.9424057268	-0.5857552819

H	1.5344330150	-5.5682367581	-2.6887147659
C	-1.8740902985	-3.0257931306	-1.3634195734
H	0.4157276845	-6.2449296533	-1.4934224557
H	-2.7406953446	-2.9883640182	-0.7172332133
H	3.5787031862	-1.4496424267	-1.8324646407
S	-1.4341057416	1.6150729535	0.4049373051
C	2.7005626465	-0.8549539888	-1.6230714407
S	1.5772675745	-1.4771682443	-0.4197145530
C	0.5193201537	-0.0681410231	-0.4954374909
C	-0.5137909854	0.1119114384	0.3548502318
H	-3.2315398048	1.7793241575	2.0707995568
H	3.0172835469	0.7862318453	-2.9624809441
C	2.4098640189	0.3041613013	-2.2085612414
C	-2.4876368506	1.0818315577	1.7082164789
S	0.9096133040	1.0978757870	-1.7593508668
S	-1.0643815531	-1.1453896655	1.4637332297
C	-2.3198265578	-0.1505149599	2.1810022157
H	-2.9167516515	-0.5971611747	2.9633151718
N	2.8019911862	3.7465086350	-2.2025151959
C	3.0535317028	4.1047538786	-3.2652958306
N	-4.1485032381	-2.6677285625	1.1012704183
C	-4.6815224096	-3.2636449133	1.9262299702
C	-5.3556874886	-4.0192728007	2.9714636859
H	-5.7764401359	-4.9295038360	2.5449976370
H	-4.6405303289	-4.2793338602	3.7509230475
H	-6.1551902242	-3.4146610264	3.3976704365
C	3.3755848596	4.5634125325	-4.6090546117
H	4.4556239579	4.5438224601	-4.7506434609
H	2.9016676755	3.9107116639	-5.3412141984
H	3.0132777430	5.5828247092	-4.7397579097

## S2.2 TTF ⊂ CBPQT<sup>4+</sup> Side-On Complex-2CH<sub>3</sub>CN

M06-2X/6-311G\*\* in PCM: -3698.3728296208

M06-2X/6-311G(2df,p) in PCM: -3698.5270797703

H	4.7881912934	6.2760816213	-4.2475270293
H	3.7325023914	5.9325979502	-2.8656153302
H	3.6930184754	3.7848604613	-1.9322471651
C	4.6023451756	3.5222059762	-2.4567842056
H	8.5250634636	0.9748156696	-4.4257530026
H	9.4109641447	-1.3035227111	-4.2376358413
H	4.9012790078	1.7119733703	-1.4273333817
N	5.0171976786	4.3751151490	-3.4117549238
H	9.7046375036	-3.2282446847	-2.9389558057
C	5.2886310637	2.3580404120	-2.2013919532
C	8.1339894146	0.3329166499	-3.6496507161
C	8.6559973041	-0.9371394178	-3.5545795308

H	8.5221619630	-3.6402607952	-1.6848484512
C	6.1514258400	4.1363051476	-4.0922239288
C	6.4250026460	2.0326639572	-2.9529195951
C	6.8681011782	2.9757829757	-3.8895089553
C	7.1013978899	0.7305795624	-2.7908498535
H	6.4562139650	4.8867224765	-4.8106304323
H	7.7615525029	2.8360851927	-4.4805028673
N	8.2017704090	-1.8051065109	-2.6323598407
C	6.7092341257	-0.1718394716	-1.7935938533
H	5.9656049711	0.0698996370	-1.0482062687
C	7.2805827186	-1.4243793263	-1.7307762440
C	4.1465268440	5.5286160127	-3.7875912531
H	7.0264188113	-2.1470010250	-0.9654016187
C	8.6461507851	-3.2288275032	-2.6849141021
C	3.0824411757	5.0343869643	-4.7344768991
H	4.3043613363	5.2906435944	-6.4948511134
C	7.8119581985	-3.9442831369	-3.7179740073
H	1.6043820871	4.7410584846	-3.1971338152
H	9.2725151115	-3.7260336705	-5.2839691198
H	6.1940751648	-4.3854120530	-2.3604096008
C	3.3648588714	4.9217835520	-6.0965695179
C	1.8476513788	4.6195988718	-4.2471753118
C	8.2717043471	-4.0543125567	-5.0254984249
C	6.5407408624	-4.4166730693	-3.3884488023
H	11.9517854480	0.0907140644	-1.8187983506
S	7.5758482354	4.5296881872	-0.8013893368
C	11.2294328709	0.8948038179	-1.8344156757
S	9.8935156879	0.7845054068	-0.6998270913
C	9.1950113130	2.3430077465	-1.1455854263
C	8.1492703044	2.8904431937	-0.4873180158
H	5.8352996640	5.4333149067	0.6554642739
H	12.0514856803	2.1477310296	-3.3685633486
C	11.2863074166	1.9593972522	-2.6284655540
C	6.3977229329	4.5232304547	0.5006404837
S	10.0223290018	3.1687297951	-2.4680528389
S	7.3017799361	2.0512379309	0.8142050187
C	6.2748338142	3.4152358843	1.2245239612
H	5.5880637483	3.2841584212	2.0488829764
C	2.4371160241	4.3448926956	-6.9513978083
C	0.9163994859	4.0434367750	-5.1043381958
C	7.4482840305	-4.5847472804	-6.0121775102
C	5.7164581334	-4.9417626852	-4.3732972327
H	2.6588089151	4.2673564080	-8.0105258222
H	-0.0444080835	3.7230415763	-4.7164585953
H	7.8150008212	-4.6636737019	-7.0299202598
C	1.2201467273	3.8792401784	-6.4519155246

H	4.7276997650	-5.3015109516	-4.1063170799
C	6.1607691915	-5.0046179383	-5.6949099381
C	0.2869486979	3.1106728633	-7.3541645516
H	1.6826592956	2.0829638856	-9.2966494880
C	5.2185935529	-5.4371033397	-6.7906380459
C	1.5779296239	1.3611409922	-8.4983045984
N	0.8020859844	1.7116776911	-7.4567975065
H	0.2505517182	3.5127482221	-8.3650973830
H	5.8364970433	-3.3264864258	-8.1070576862
C	2.1981936753	0.1303631872	-8.5245214942
H	-0.7266942371	3.0542895777	-6.9604751874
C	0.5961329699	0.8704008099	-6.4297471442
H	2.7995122062	-0.1228915485	-9.3871574287
C	4.8180807340	-3.2357766434	-7.7559823479
N	4.3092428558	-4.2890725652	-7.0952381150
H	-0.0393539150	1.2230119475	-5.6283782642
C	2.0365553920	-0.7453455363	-7.4495234280
C	4.0753285369	-2.0900415947	-7.9275958234
C	1.1956908792	-0.3697458650	-6.4028598625
C	2.7935506966	-2.0168092987	-7.3850823186
H	4.5387676254	-1.2570870105	-8.4385918968
C	3.0520982828	-4.2719512793	-6.6129529295
H	1.0371783230	-0.9968405062	-5.5361579763
H	2.7024060015	-5.1883161161	-6.1592773016
H	5.7492694761	-5.6786372675	-7.7090102677
C	2.2706141898	-3.1421581414	-6.7437928249
H	4.5926298832	-6.2799076968	-6.5034540681
H	1.2594139024	-3.1595626962	-6.3585440772
C	4.1935525623	1.5515450189	-5.6454453702
N	3.4004904322	1.4800589193	-4.8144972593
C	5.2050851758	1.6307902153	-6.6921396512
H	5.5149779395	2.6661436535	-6.8310621423
H	6.0633882407	1.0137592908	-6.4206054533
H	4.7934075683	1.2678447165	-7.6333726012
N	5.8709081818	-1.4269900572	-5.3008247846
C	5.0289536258	-1.5271137276	-4.5225971758
C	3.9564312844	-1.6305340887	-3.5400443826
H	3.6535378359	-0.6277469601	-3.2352369420
H	3.0988456372	-2.1437149745	-3.9752593949
H	4.2966926081	-2.1954021537	-2.6724586217

### 2.3 TTF $\subset$ CBPQT<sup>4+</sup> Side-On Complex-2CH<sub>3</sub>CN

M06-2X/6-311G\*\* in PCM: -3432.867612915

H	5.0401336287	6.2495420321	-4.5377000485
H	3.9335787278	5.9361578252	-3.1899230495
H	3.9908421071	3.9642100238	-2.0596367560

C	4.8272813452	3.5943232967	-2.6355995233
H	9.0391195619	1.1145273966	-4.0132685248
H	9.9111202230	-1.1812446745	-3.7834578298
H	5.1440010081	1.8561996784	-1.4842346484
N	5.2144813338	4.3567721000	-3.6747155232
H	9.7667012645	-3.2593594052	-3.1014437474
C	5.4881214449	2.4247828937	-2.3374796638
C	8.4479490208	0.3838816887	-3.4770233003
C	8.9556684515	-0.8932690778	-3.3687742166
H	8.6921600108	-3.6616673232	-1.7515239956
C	6.2860183316	4.0159942810	-4.4150152742
C	6.5669073224	2.0065059331	-3.1245087390
C	6.9812097269	2.8579261287	-4.1582989140
C	7.2058464452	0.6941111026	-2.9154188653
H	6.5463232871	4.6819873056	-5.2264924597
H	7.8044204912	2.6149236291	-4.8160270833
N	8.2733491712	-1.8508544480	-2.7179907256
C	6.5570577091	-0.3121953472	-2.1838092736
H	5.5953208421	-0.1573951945	-1.7158715801
C	7.1046096140	-1.5689183127	-2.1088492338
C	4.3726974247	5.5150150737	-4.0929175117
H	6.6126389605	-2.3859170287	-1.5975578265
C	8.7306285163	-3.2697954634	-2.7670014640
C	3.3332754799	5.0259211502	-5.0732991221
H	4.4620200925	5.5994279478	-6.8158198007
C	7.8212502760	-4.0307803832	-3.7018556151
H	1.9427243503	4.3979444992	-3.5495609540
H	8.6399492677	-3.1320308659	-5.4864691466
H	6.8395851054	-5.1257933471	-2.1346974524
C	3.5760057731	5.0977860737	-6.4423124296
C	2.1634953138	4.4225165414	-4.6106371489
C	7.8767925944	-3.7853855106	-5.0761982260
C	6.8661105368	-4.9048200718	-3.1954349128
H	12.2122258096	1.8500980639	-2.8413941883
S	6.9867912805	3.8478343908	0.1087289807
C	11.3198405346	2.3258531012	-2.4580601429
S	10.4318140676	1.4644323624	-1.2159149578
C	9.1503782965	2.6683359428	-1.0902804698
C	8.1078482558	2.5317782126	-0.2374611238
H	5.1523629175	3.4104601556	1.6614095284
H	11.3213635050	4.1546406178	-3.5773995747
C	10.8577310822	3.5141123236	-2.8397609002
C	6.0097569531	2.9148161442	1.2271025314
S	9.3975043432	4.1119392610	-2.0744478971
S	7.8317349797	1.0626433989	0.7007019157
C	6.3906828032	1.6682285187	1.4942175501



H	5.8929221173	0.9992501583	2.1829748875
C	2.6830377753	4.5252368467	-7.3416752809
C	1.2745123476	3.8479695289	-5.5072589523
C	6.9450545392	-4.3620182970	-5.9229682843
C	5.9281143384	-5.4845476487	-4.0469250572
H	2.8779882210	4.5900212784	-8.4063534684
H	0.3730757302	3.3750282043	-5.1336373601
H	6.9854171721	-4.1561363455	-6.9873735725
C	1.5445644914	3.8730857076	-6.8753450657
H	5.1760037298	-6.1536304860	-3.6435334083
C	5.9463144989	-5.1907621526	-5.4057246401
C	0.6498929403	3.1243679996	-7.8329570029
H	2.5680445860	2.0392291673	-9.1820692640
C	4.8425900806	-5.6810546045	-6.3101261628
C	2.1155034718	1.2962113372	-8.5374984698
N	1.0436438541	1.6823249959	-7.8226244067
H	0.7512972999	3.4785941508	-8.8574817135
H	4.4417827845	-4.6852937988	-8.6942922567
C	2.6179569947	0.0199367629	-8.4164638480
H	-0.4000305087	3.1690260664	-7.5496550220
C	0.4049553743	0.8238297576	-7.0082576374
H	3.5080852130	-0.2448365392	-8.9710798638
C	3.9318941665	-4.0817748977	-7.9559124625
N	3.9812963743	-4.5149003884	-6.6850557357
H	-0.4606557207	1.2056934698	-6.4863875801
C	2.0127297768	-0.8717554509	-7.5296034761
C	3.2539537274	-2.9215698650	-8.2756528523
C	0.8680466165	-0.4645810563	-6.8463858251
C	2.6276340508	-2.1941791465	-7.2662079778
H	3.2355085234	-2.5991984757	-9.3083678577
C	3.3367615890	-3.8595461268	-5.7015510555
H	0.3370083046	-1.1252891117	-6.1749244991
H	3.4236545990	-4.2705851972	-4.7038036572
H	5.2167324413	-6.1065360991	-7.2389261826
C	2.6470184132	-2.6998723811	-5.9642732636
H	4.2010180740	-6.4099420948	-5.8168811682
H	2.1826494232	-2.1724919092	-5.1425121217

## S2.4 TTF $\subset$ CBPQT<sup>4+</sup> Inclusion Complex-2CH<sub>3</sub>CN

M06-2X/6-311G\*\* in PCM: -3432.8937621033

H	5.1978338015	6.3488790130	-4.3384621221
H	4.1795386747	6.0702549025	-2.9163618479
H	4.4158846673	4.2371796466	-1.6666491597
C	5.1367349296	3.7863478338	-2.3333201103
H	9.0366772588	1.0519571712	-4.0942273364
H	9.8946218749	-1.2378379146	-3.7832637176

H	5.5889196606	2.1188815852	-1.1136462723
N	5.3834622367	4.4542233096	-3.4750495265
H	9.9256111600	-3.1957328176	-2.6691706181
C	5.7921836409	2.6052867038	-2.0574505029
C	8.5045656032	0.3827055251	-3.4324552013
C	9.0113190957	-0.8892658932	-3.2661441155
H	8.7394802572	-3.5556722328	-1.4031361466
C	6.2907852515	4.0017120510	-4.3566137696
C	6.7044994850	2.0821123481	-2.9785676577
C	6.9666838386	2.8223449385	-4.1340488772
C	7.3392697385	0.7595282147	-2.7603158503
H	6.4513394447	4.6115011838	-5.2352828483
H	7.6782637751	2.5021848341	-4.8819187129
N	8.4117158698	-1.7693266666	-2.4446550307
C	6.7515253348	-0.1729483731	-1.9009423701
H	5.8483597827	0.0447628905	-1.3503389567
C	7.3075363916	-1.4245430271	-1.7597493853
C	4.5422634007	5.6339081203	-3.8453213964
H	6.8851574748	-2.1721453773	-1.1006874546
C	8.8658807736	-3.1935441414	-2.4224452745
C	3.4256749798	5.1565834958	-4.7440034522
H	4.5490731840	5.4158502579	-6.5683281947
C	8.0413476131	-3.9679494623	-3.4228044326
H	2.0139423896	4.8800910871	-3.1419535665
H	9.4897848238	-3.8008223461	-5.0086623325
H	6.4347866721	-4.3883559734	-2.0434013524
C	3.6376131214	5.0388396112	-6.1176624964
C	2.2123585274	4.7398882774	-4.1993984071
C	8.4889047016	-4.1175285544	-4.7333664737
C	6.7797425725	-4.4468821883	-3.0701081558
H	8.1837181826	-1.9496191010	-6.7879565417
S	3.5025562860	1.6975425265	-4.6290452725
C	7.3866737846	-1.2502093844	-6.5746614859
S	6.2904478188	-1.6443274621	-5.2573059635
C	5.3583224358	-0.1549584616	-5.4069101025
C	4.3398828526	0.1451575887	-4.5736256284
H	1.7603211640	2.0947983663	-2.9426441890
H	7.7933773239	0.2461737643	-8.0537498989
C	7.1880168478	-0.1106457087	-7.2308432474
C	2.4540457566	1.3298145238	-3.2662043393
S	5.8389595283	0.8998992746	-6.7403741409
S	3.7337020392	-0.9943435237	-3.3656757661
C	2.5639377425	0.1329858491	-2.6980235815
H	1.9746521923	-0.2103293333	-1.8577781699
C	2.6814210359	4.4331572276	-6.9217820576
C	1.2514285262	4.1358194144	-5.0067941519

C	7.6538796699	-4.6740713343	-5.6995841895
C	5.9475454504	-5.0004712582	-4.0330516414
H	2.8619149569	4.3451823799	-7.9872904381
H	0.3077182469	3.8141003750	-4.5793552042
H	8.0118859337	-4.7842048104	-6.7182959030
C	1.5012571238	3.9425414118	-6.3644657124
H	4.9648984577	-5.3533305147	-3.7390965108
C	6.3663783156	-5.0834433444	-5.3606397423
C	0.5565166137	3.1207513321	-7.2103037564
H	2.1430958796	2.1056324040	-9.0030102493
C	5.3981590166	-5.5263183739	-6.4322001170
C	1.9669569882	1.3831025886	-8.2170644768
N	1.0761708727	1.7200859569	-7.2680178376
H	0.4963697206	3.4800530485	-8.2361884739
H	5.8192962741	-3.6736684655	-8.1766200201
C	2.5994948519	0.1589649689	-8.1884100777
H	-0.4485194940	3.0745032689	-6.7936653173
C	0.7761423956	0.8629012500	-6.2772583391
H	3.2871937252	-0.0635382555	-8.9914153061
C	4.9064928057	-3.4523682284	-7.6396962325
N	4.4975772106	-4.3779569767	-6.7549627942
H	0.0480911802	1.1943592786	-5.5480817763
C	2.3288328776	-0.7460599399	-7.1571979155
C	4.2048901583	-2.2792058283	-7.8157826217
C	1.3795896298	-0.3743726854	-6.2013789952
C	3.0540882336	-2.0368398736	-7.0609613261
H	4.6012962978	-1.5629165689	-8.5225307849
C	3.3704261144	-4.1947849938	-6.0442379219
H	1.1157740733	-1.0091945629	-5.3671246326
H	3.0933114649	-4.9857170680	-5.3624962356
H	5.9119893841	-5.8032500891	-7.3497780444
C	2.6293566242	-3.0408445973	-6.1838853504
H	4.7743257891	-6.3564213571	-6.1067525453
H	1.7266676322	-2.9569327299	-5.5952218474

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 [2] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.